libEnsemble: A Library for Managing Dynamic Ensembles of Calculations

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- A `libEnsemble` worker is the smallest indivisible unit to perform

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`sim_f`: Evaluates a simulation (i.e., user-defined function) using input defined by `gen_f`

`alloc_f`: Decides whether (or not) `sim_f` or `gen_f` should be called (and with what input/resources) as workers become available

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- Python 3.5+, NumPy, psutil

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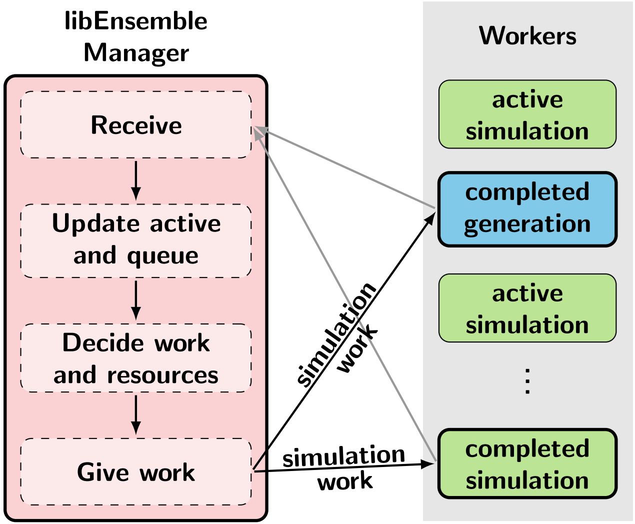
- Example `gen_f`/`sim_f` functions require NLopt, PETSc, SciPy, Tasmanian, etc.

`libEnsemble` overview



libEnsemble Manager

Receive

Update active and queue

Decide work and resources

Give work

Workers

active simulation

completed generation

active simulation

⋮

completed simulation

Possible user requirements of `libEnsemble`

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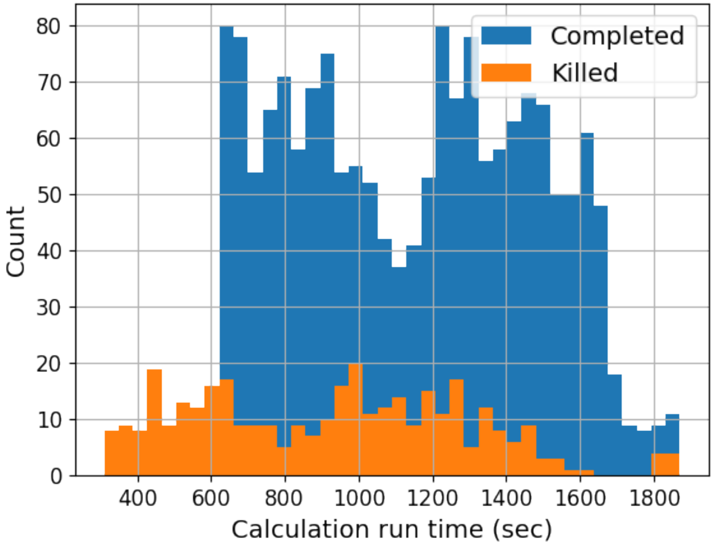
- Thousands of concurrent workers

OPAL particle accelerator simulations on 1024 Theta nodes



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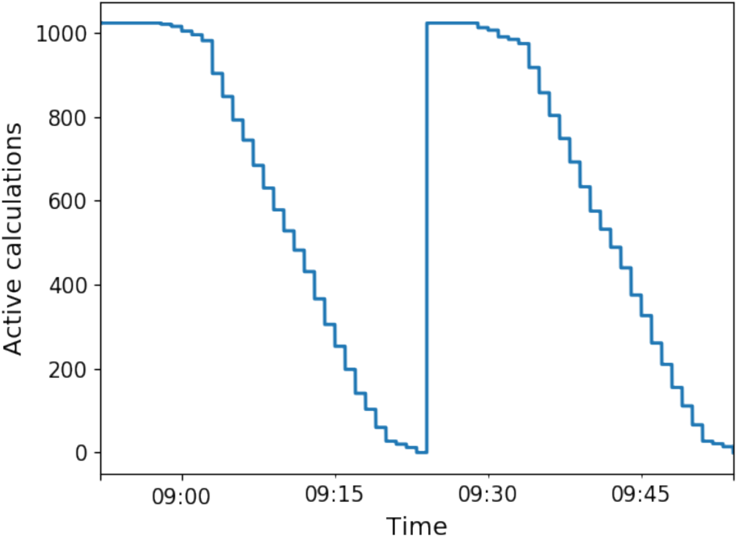

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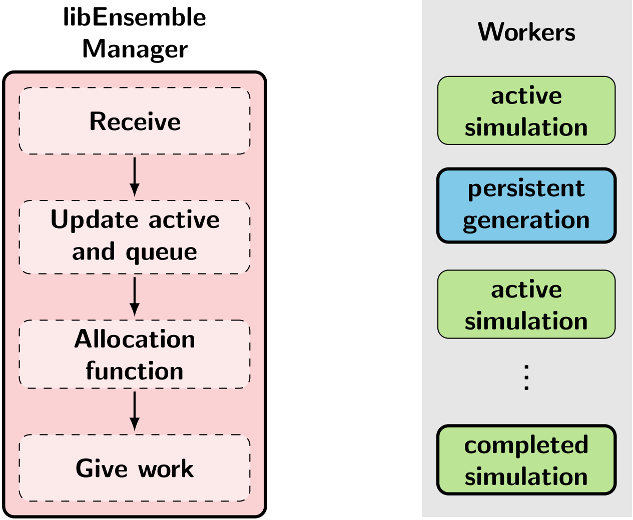
- Don't have to write your own kills, just complete `libEnsemble` templates
- Want to add concurrency to a generator (e.g., multiple local optimizers.)

Why `libEnsemble` and not. . . ?

Swift: (the parallel scripting language)

- “Can run million programs, thousands at a time, launching hundreds per second”
- Require writing your generators in Swift’s scripting language
- Difficult to tightly couple generation of inputs and future/active running simulations

libEnsemble overview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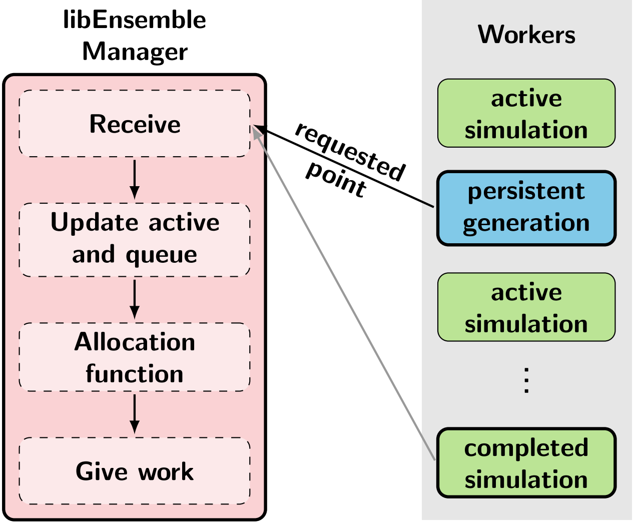

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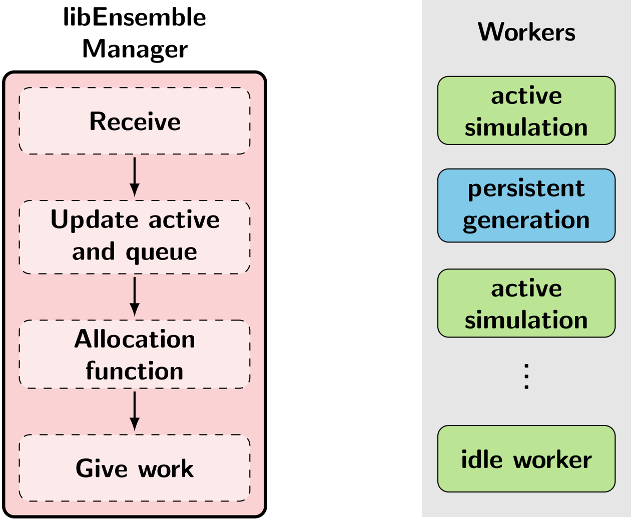

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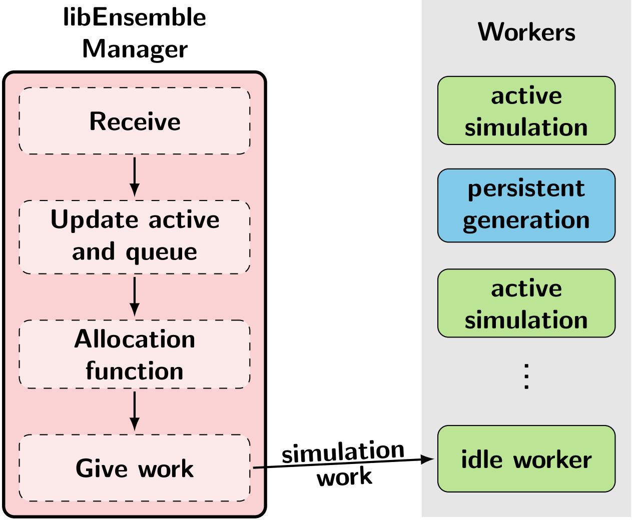

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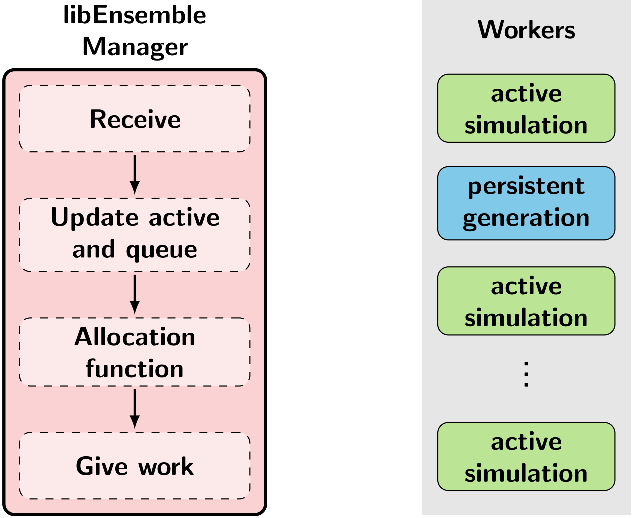

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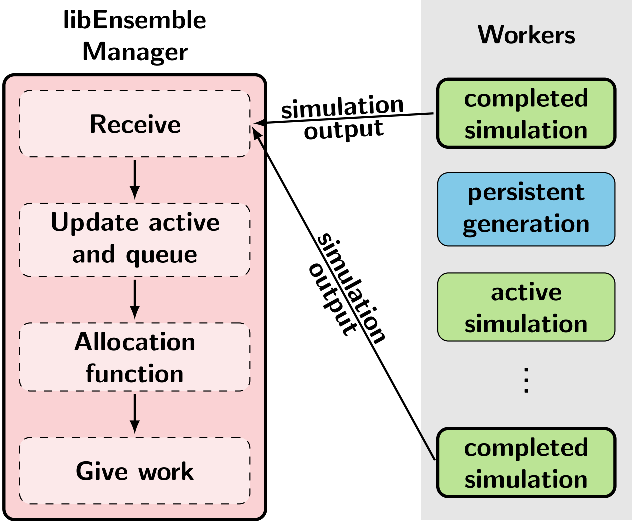

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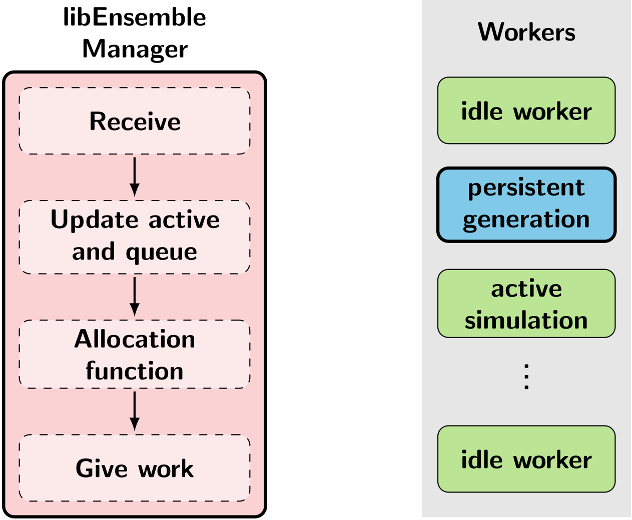

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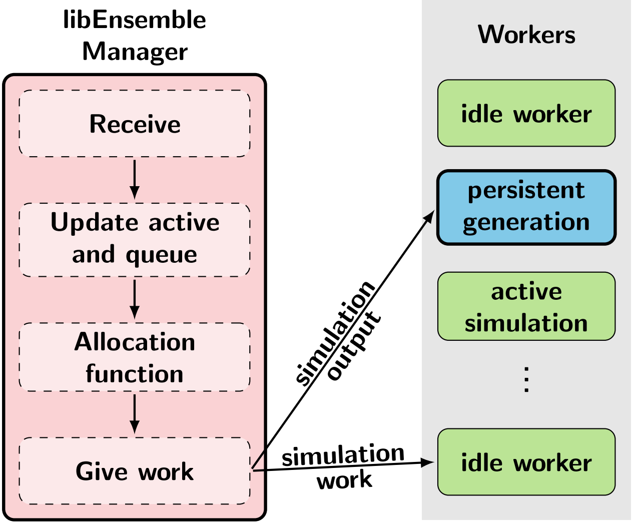
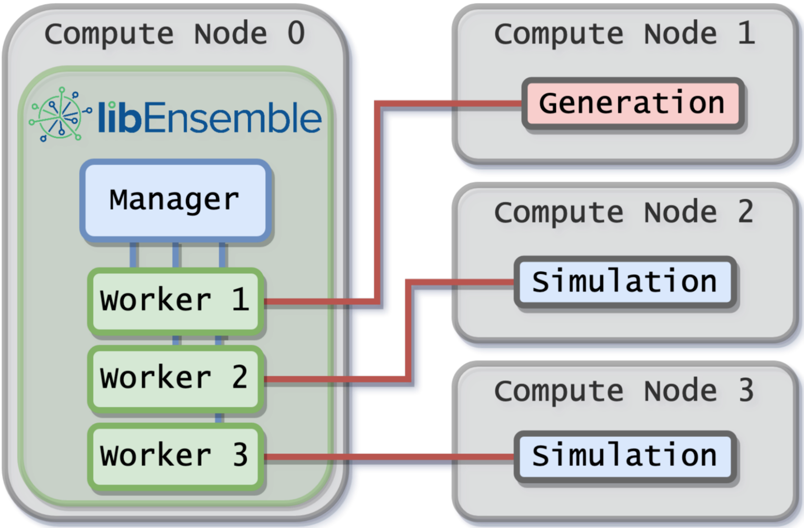


libEnsemble modes: centralized or distributed



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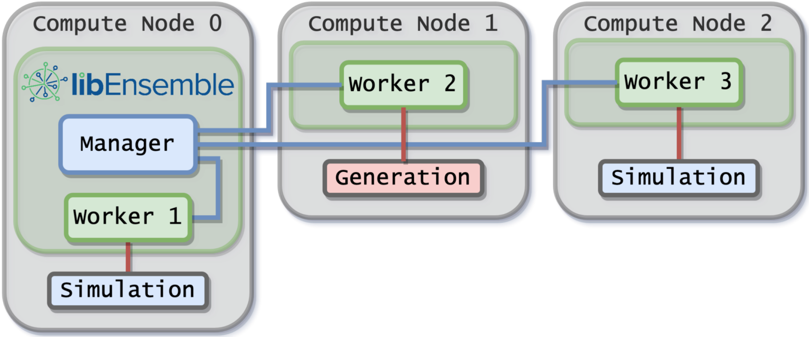

Timing `libEnsemble` overhead

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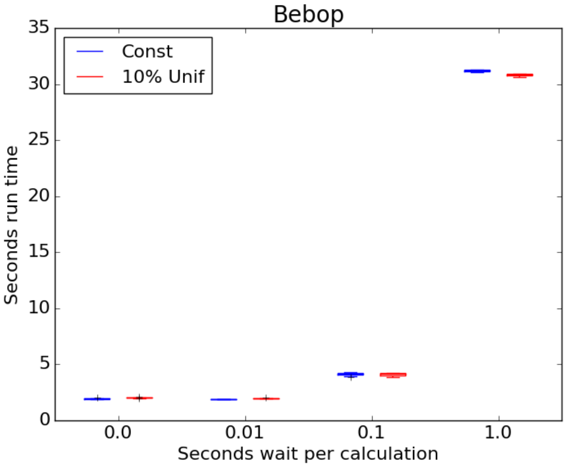
- Tons of system-dependent caveats
- 32 nodes × 36 cores = 1152-1 workers



Use cases

- A user wants to optimize a function that depends on a simulation
- The simulation is already using parallel resources, but not a large fraction of some computer
- `libEnsemble` can coordinate the concurrent evaluation of the simulation `sim_f` at various parameter values and `gen_f` would return candidate parameter values (possibly after each `sim_f` output)

Use cases

- A user has a `gen_f` that produces different meshes to be used within a `sim_f`
- Given the `sim_f` output, `gen_f` will refine a mesh or produce a new mesh
- `libEnsemble` can ensure that the calculated meshes can be used by multiple simulations without requiring movement of data

Use cases

- A user wants to evaluate a simulation `sim_f` at parameters sampled from a set of parameter values
- Many parameter sets will cause the simulation to fail
- `libEnsemble` can stop unresponsive evaluations, and recover computational resources for future evaluations
- `gen_f` can update the sampling after discovering regions where evaluations of `sim_f` fail

Use cases

- A user has a simulation `sim_f` that requires calculating multiple expensive quantities, some of which depend on other quantities
- `libEnsemble` can observe intermediate quantities in order to stop related calculations and preempt future calculations associated with a poor parameter values

Use cases

- A user wishes to identify multiple local optima for a `sim_f`
- `libEnsemble` can use the points from the APOSMM `gen_f` to identify optima

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Naturally, combinations of use cases is supported as well

Problem setup

- We want to identify distinct, “high-quality”, local minimizers of

$$\begin{aligned} \text{minimize}\, f(x) \\ l \leq x \leq u \\ x \in \mathbb{R}^n \end{aligned}$$

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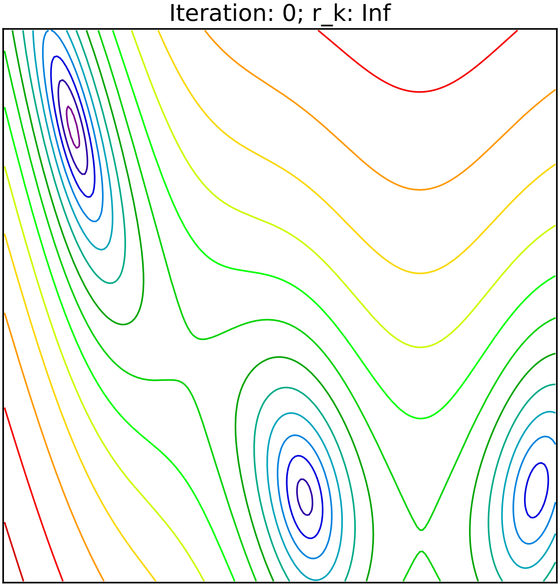
- Possibly have a specialized local optimization method for f

APOSMM



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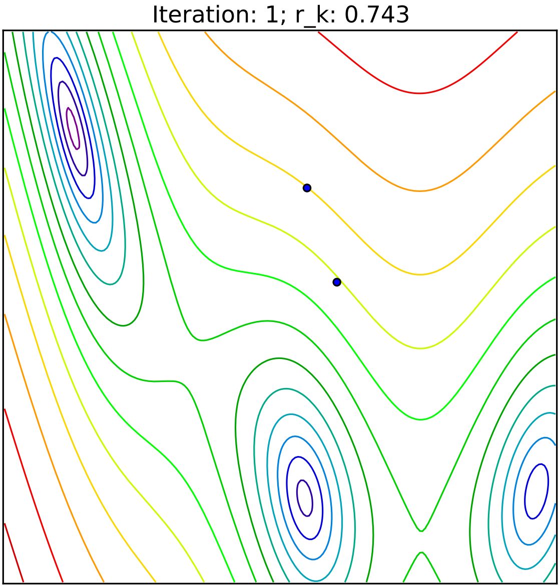

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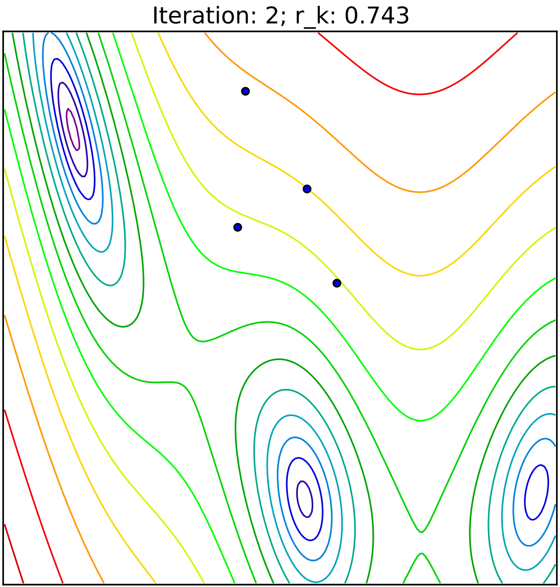

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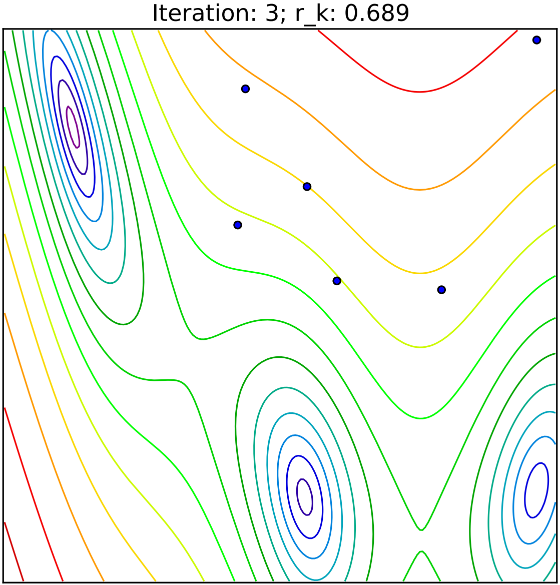
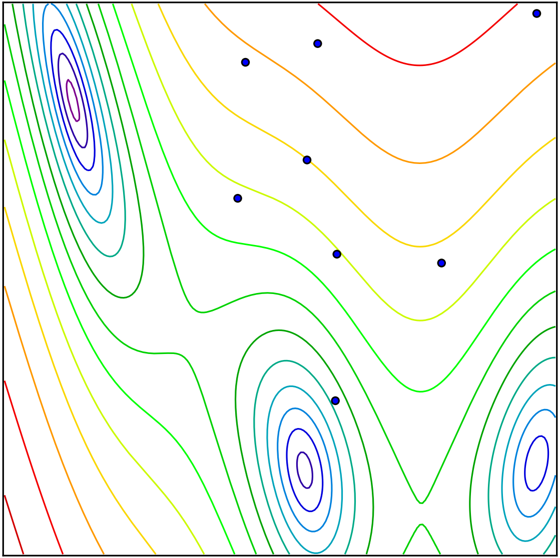


APOSMM

Iteration: 4; r_k: 0.643



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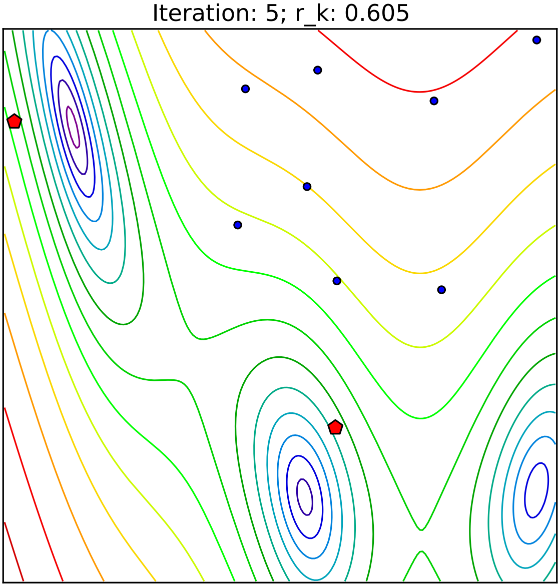

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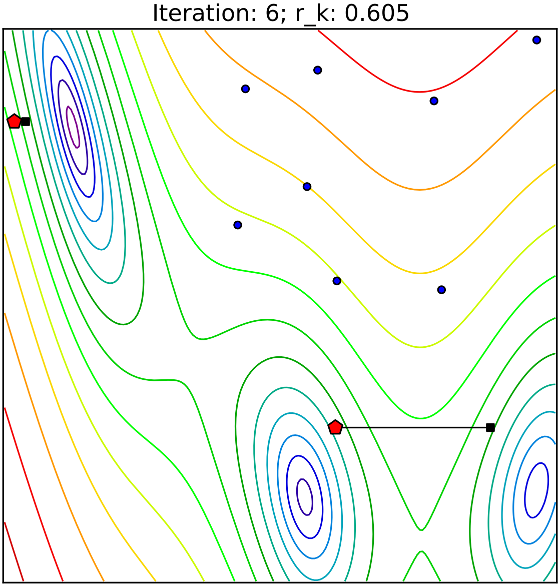

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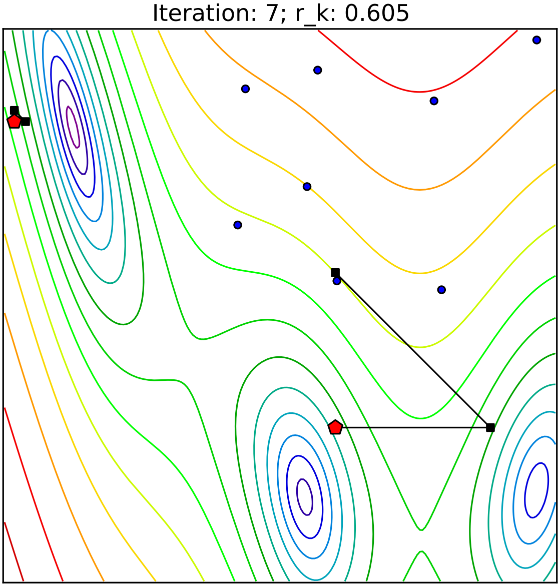

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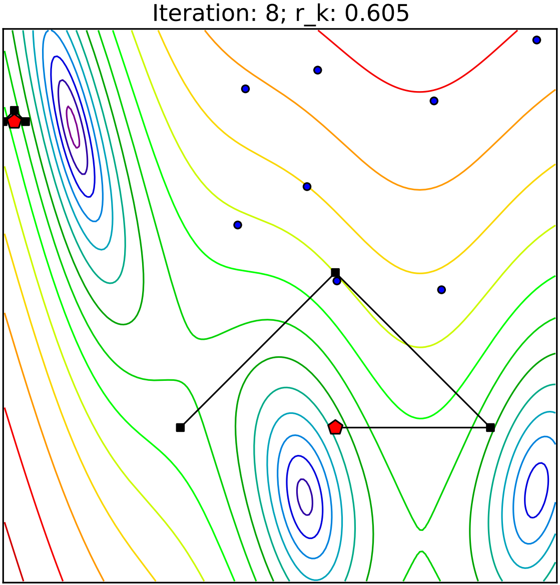

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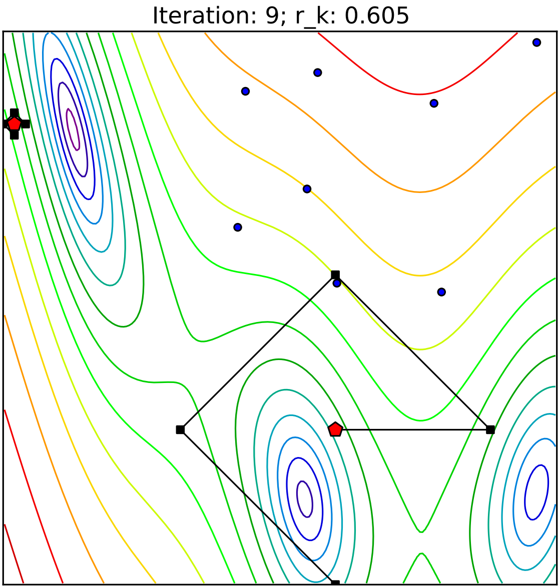

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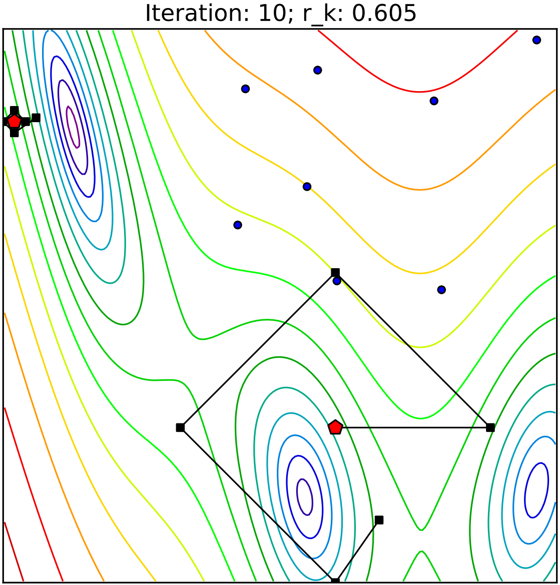

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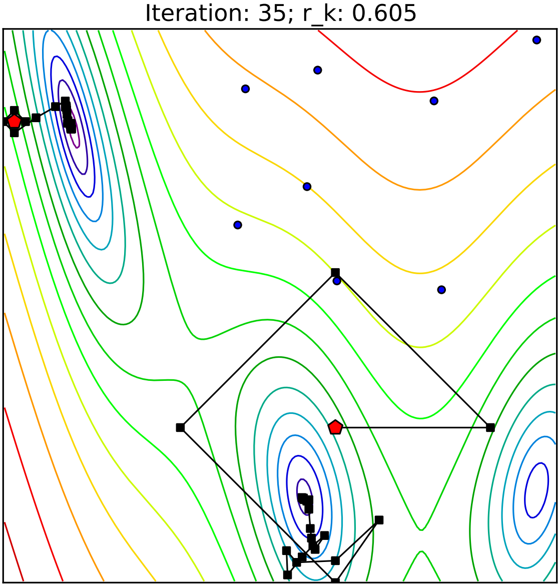

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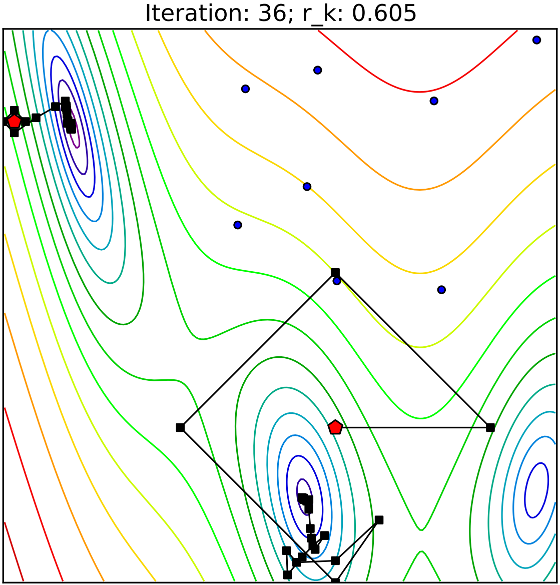

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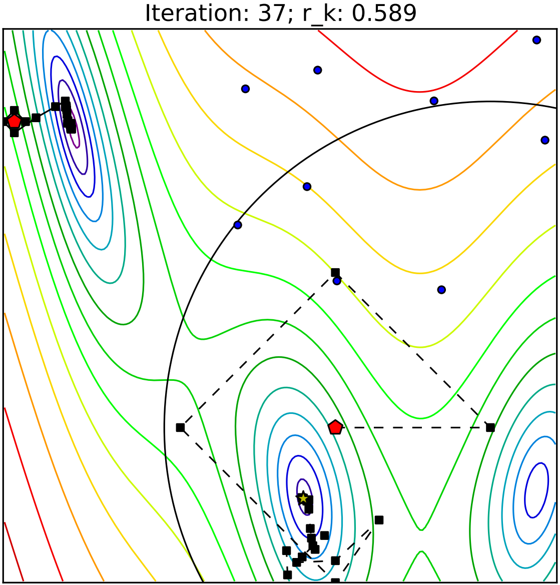

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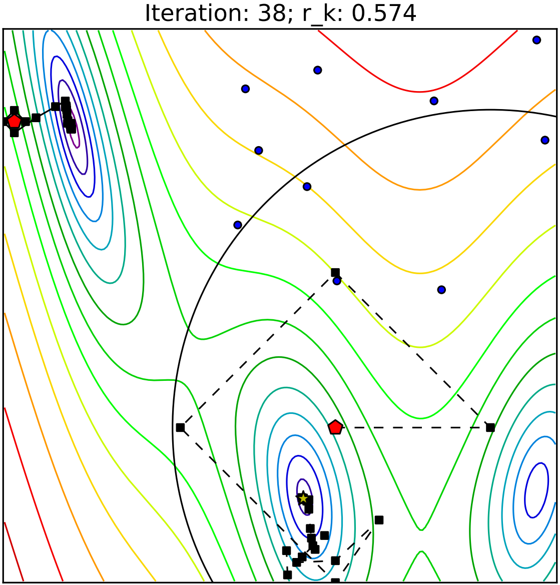

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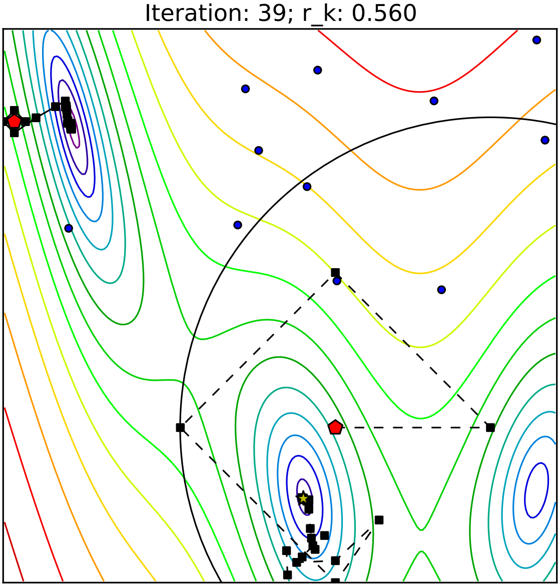

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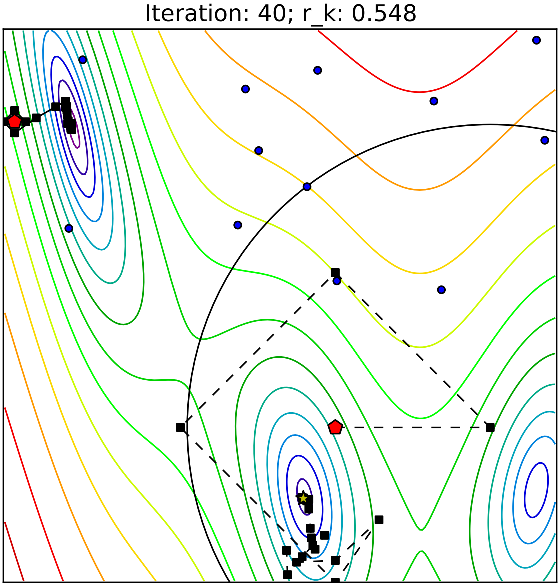

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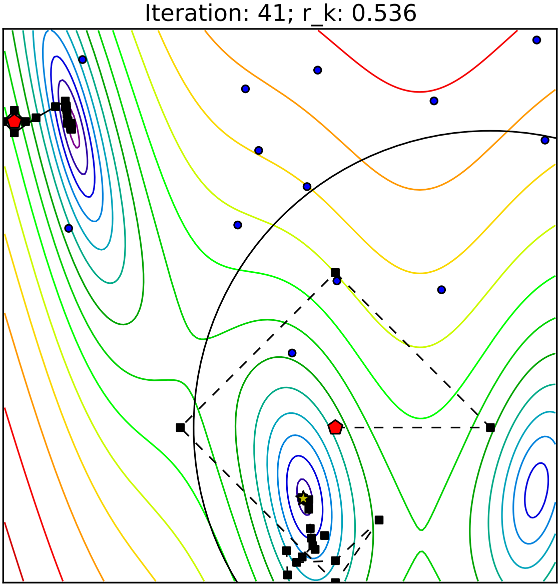
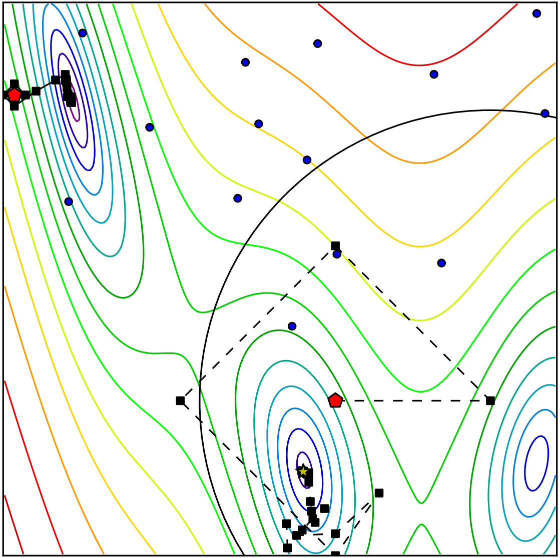


APOSMM

Iteration: 42; r_k: 0.525



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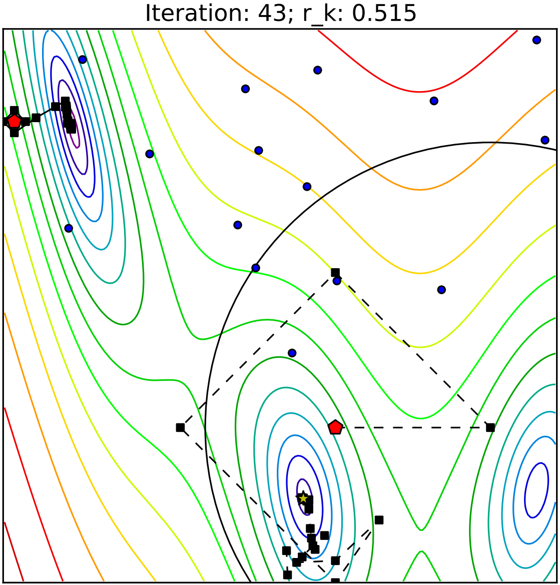

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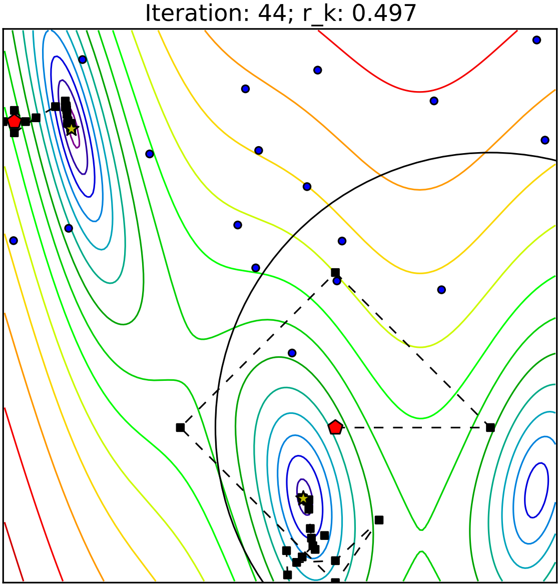

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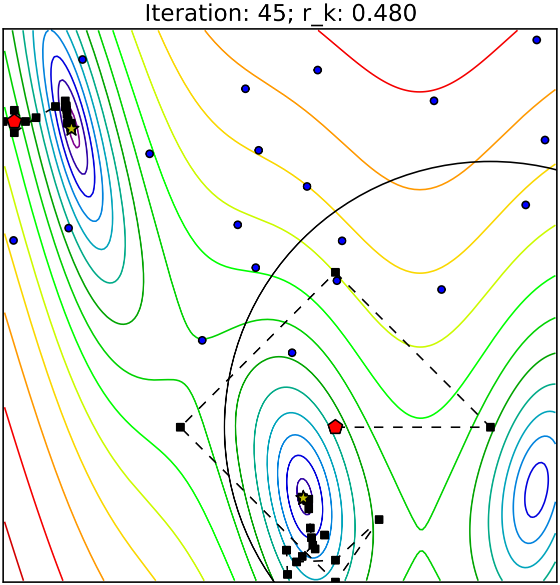

Closing Remarks

- We have a growing set of use cases and examples
- Let us know if you have examples you'd like to see
- `https://github.com/Libensemble/libensemble`